Full wwPDB X-ray Structure Validation Report

Sep 14, 2020 – 07:25 AM BST

PDB ID	:	6SRX
Title	:	Structure of the arginase-2-inhibitory human antigen-binding fragment Fab C0021158
Authors	:	Burschowsky, D.; Addyman, A.; Fiedler, S.; Groves, M.; Haynes, S.; Seewooruthun, C.; Carr, M.
Deposited on	:	2019-09-06
Resolution	:	1.90 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 following versions of software and data (see references (1)) were used in the production of this report:

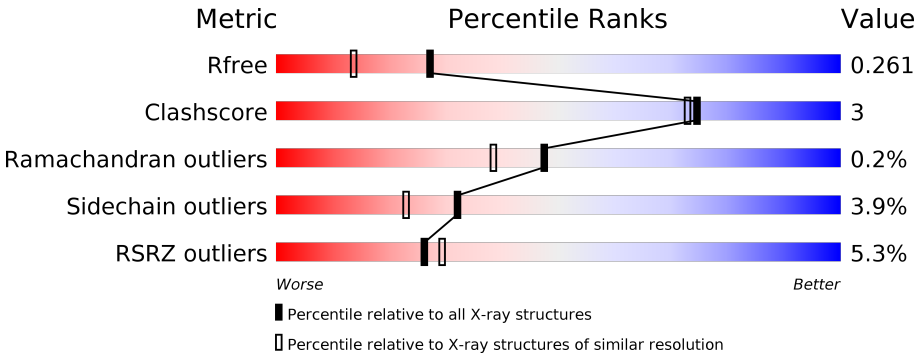
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.4.dev1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.4.dev1

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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 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	HHH	233	3% 85% 9% • 5%
1	III	233	3% 83% 11% • 5%
2	LLL	220	5% 90% 6% •
2	MMM	220	9% 89% 7% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13202 atoms, of which 6400 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.

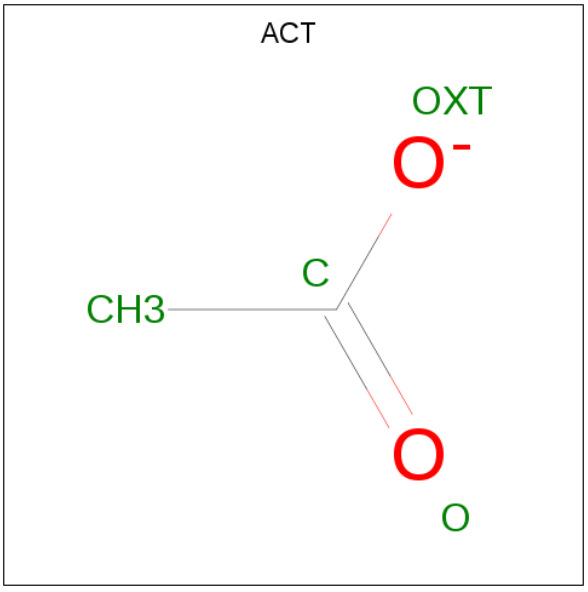
- Molecule 1 is a protein called Fab C0021158 heavy chain (IgG1).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	HHH	221	Total	C	H	N	O	S	88	3	0
			3335	1056	1662	288	321	8			
1	III	221	Total	C	H	N	O	S	88	3	0
			3335	1056	1662	288	321	8			

- Molecule 2 is a protein called Fab C0021158 light chain (IgG1).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	LLL	213	Total	C	H	N	O	S	102	0	0
			3110	987	1532	261	326	4			
2	MMM	212	Total	C	H	N	O	S	102	1	0
			3110	987	1532	261	326	4			

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	HHH	1	Total C H O 7 2 3 2	0	0
3	HHH	1	Total C H O 7 2 3 2	0	0
3	III	1	Total C H O 7 2 3 2	0	0
3	III	1	Total C H O 7 2 3 2	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	HHH	1	Total Cl 1 1	0	0
4	III	1	Total Cl 1 1	0	0

- Molecule 5 is water.

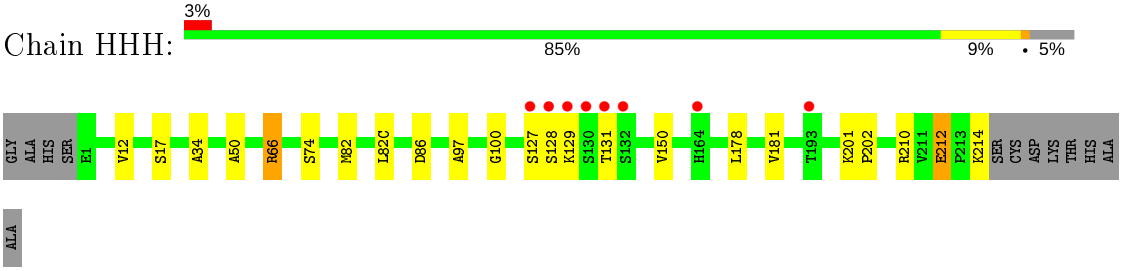
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	HHH	88	Total O 88 88	0	0
5	LLL	57	Total O 57 57	0	0
5	III	89	Total O 89 89	0	0
5	MMM	48	Total O 48 48	0	0

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.

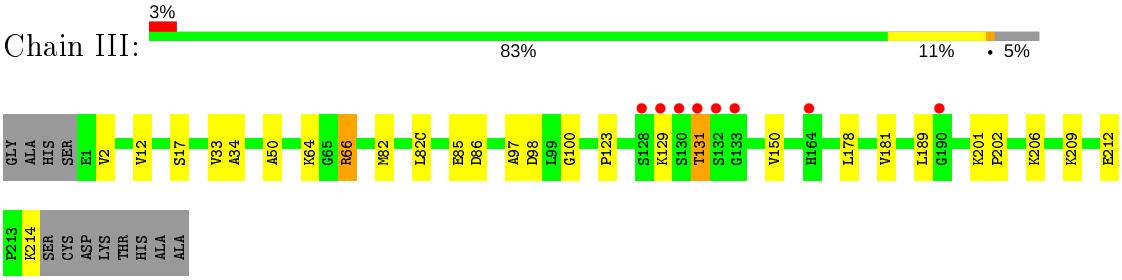
- Molecule 1: Fab C0021158 heavy chain (IgG1)

Chain HHH:



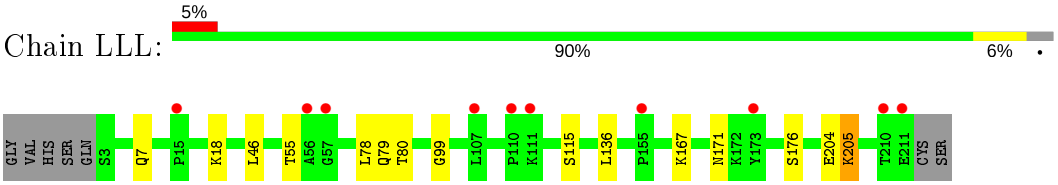
- Molecule 1: Fab C0021158 heavy chain (IgG1)

Chain III:



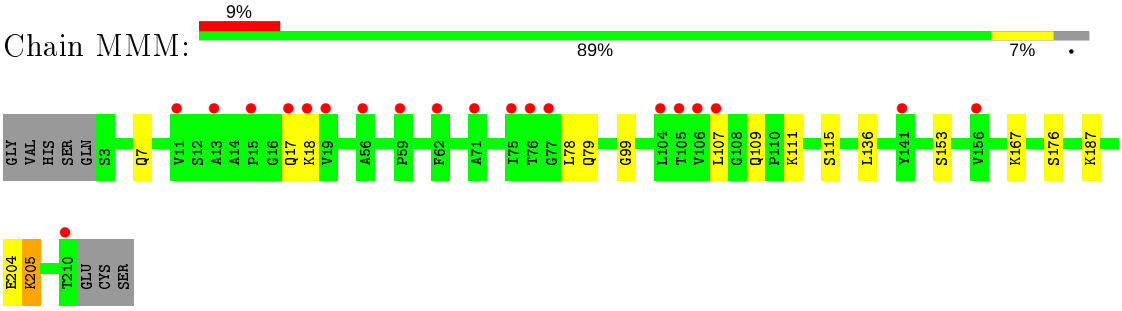
- Molecule 2: Fab C0021158 light chain (IgG1)

Chain LLL:



- Molecule 2: Fab C0021158 light chain (IgG1)

Chain MMM:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.73Å 122.67Å 63.98Å 90.00° 114.89° 90.00°	Depositor
Resolution (Å)	48.95 – 1.90 48.96 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.95-1.90) 98.2 (48.96-1.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.234 , 0.261 0.238 , 0.261	Depositor DCC
R_{free} test set	3129 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å^2)	30.8	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 29.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13202	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, ACT

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	HHH	0.64	0/1712	0.81	2/2330 (0.1%)
1	III	0.63	0/1712	0.82	2/2330 (0.1%)
2	LLL	0.65	0/1616	0.76	0/2210
2	MMM	0.65	0/1616	0.76	0/2210
All	All	0.64	0/6656	0.79	4/9080 (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	III	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	III	66	ARG	NE-CZ-NH2	6.36	123.48	120.30
1	HHH	66	ARG	NE-CZ-NH1	-6.16	117.22	120.30
1	HHH	66	ARG	NE-CZ-NH2	6.03	123.32	120.30
1	III	66	ARG	NE-CZ-NH1	-5.41	117.59	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	III	33	VAL	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	HHH	1673	1662	1658	15	0
1	III	1673	1662	1658	15	0
2	LLL	1578	1532	1528	14	1
2	MMM	1578	1532	1527	7	1
3	HHH	8	6	6	0	0
3	III	8	6	6	0	0
4	HHH	1	0	0	0	0
4	III	1	0	0	0	0
5	HHH	88	0	0	1	0
5	III	89	0	0	0	0
5	LLL	57	0	0	1	0
5	MMM	48	0	0	1	0
All	All	6802	6400	6383	41	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 3.

All (41) 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:III:181:VAL:HG21	2:MMM:136:LEU:CD1	2.18	0.74
1:III:66:ARG:NH1	1:III:86:ASP:OD1	2.24	0.69
1:HHH:181:VAL:HG21	2:LLL:136:LEU:CD1	2.26	0.65
1:III:181:VAL:HG21	2:MMM:136:LEU:HD13	1.78	0.65
1:HHH:66:ARG:NH1	1:HHH:86:ASP:OD1	2.24	0.64
1:III:131:THR:HG23	1:III:189:LEU:HD12	1.87	0.55
1:HHH:178:LEU:HD12	1:HHH:178:LEU:C	2.26	0.55
1:III:178:LEU:HD12	1:III:178:LEU:C	2.28	0.54
1:HHH:181:VAL:HG21	2:LLL:136:LEU:HD13	1.90	0.53
2:LLL:167:LYS:HE2	2:LLL:171:ASN:HA	1.91	0.52
2:MMM:109:GLN:O	5:MMM:301:HOH:O	2.19	0.52
2:LLL:167:LYS:HE2	2:LLL:171:ASN:HD22	1.75	0.51
1:HHH:210:ARG:HD3	1:HHH:212:GLU:OE2	2.09	0.51
1:III:123:PRO:HD3	1:III:209:LYS:HE2	1.92	0.50
2:LLL:167:LYS:CE	2:LLL:171:ASN:HD22	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:III:181:VAL:CG2	2:MMM:136:LEU:CD1	2.90	0.47
2:LLL:7:GLN:OE1	2:LLL:99:GLY:HA3	2.14	0.47
1:III:181:VAL:CG2	2:MMM:136:LEU:HD13	2.44	0.47
2:LLL:80:THR:HG23	5:LLL:347:HOH:O	2.15	0.46
2:MMM:7:GLN:OE1	2:MMM:99:GLY:HA3	2.17	0.45
1:III:12:VAL:HG11	1:III:82(C):LEU:HD13	1.99	0.45
1:HHH:181:VAL:CG2	2:LLL:136:LEU:CD1	2.93	0.45
1:HHH:97:ALA:HA	1:HHH:100:GLY:O	2.16	0.45
1:III:97:ALA:HA	1:III:100:GLY:O	2.16	0.44
1:III:34:ALA:O	1:III:50:ALA:HA	2.18	0.44
1:HHH:34:ALA:O	1:HHH:50:ALA:HA	2.18	0.43
1:HHH:66:ARG:HD3	5:HHH:454:HOH:O	2.17	0.43
1:HHH:12:VAL:HG11	1:HHH:82(C):LEU:HD13	1.98	0.43
2:LLL:46:LEU:HD23	2:LLL:55:THR:CG2	2.48	0.43
2:LLL:78:LEU:HD12	2:LLL:78:LEU:HA	1.92	0.42
1:HHH:74:SER:HB3	1:III:98:ASP:OD2	2.18	0.42
1:III:201:LYS:N	1:III:202:PRO:CD	2.83	0.42
1:HHH:201:LYS:N	1:HHH:202:PRO:CD	2.83	0.42
1:HHH:181:VAL:CG2	2:LLL:136:LEU:HD13	2.49	0.42
2:MMM:204:GLU:O	2:MMM:205:LYS:HD2	2.20	0.42
1:HHH:181:VAL:HG21	2:LLL:136:LEU:HD12	2.02	0.41
2:LLL:204:GLU:O	2:LLL:205:LYS:HD2	2.19	0.41
1:III:17:SER:HA	1:III:82:MET:O	2.21	0.41
2:LLL:46:LEU:HD23	2:LLL:55:THR:HG21	2.01	0.41
1:HHH:17:SER:HA	1:HHH:82:MET:O	2.21	0.40
1:III:2:VAL:O	1:III:2:VAL:HG23	2.21	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)
2:LLL:79:GLN:HE21	2:MMM:79:GLN:OE1[2_544]	1.59	0.01

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	HHH	222/233 (95%)	210 (95%)	11 (5%)	1 (0%)	29 18
1	III	222/233 (95%)	213 (96%)	8 (4%)	1 (0%)	29 18
2	LLL	211/220 (96%)	208 (99%)	3 (1%)	0	100 100
2	MMM	211/220 (96%)	206 (98%)	5 (2%)	0	100 100
All	All	866/906 (96%)	837 (97%)	27 (3%)	2 (0%)	47 38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	HHH	131	THR
1	III	131	THR

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	HHH	185/190 (97%)	179 (97%)	6 (3%)	39 30
1	III	185/190 (97%)	178 (96%)	7 (4%)	33 24
2	LLL	178/184 (97%)	174 (98%)	4 (2%)	52 47
2	MMM	178/184 (97%)	167 (94%)	11 (6%)	18 9
All	All	726/748 (97%)	698 (96%)	28 (4%)	32 23

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	HHH	127	SER
1	HHH	128	SER
1	HHH	129	LYS
1	HHH	150	VAL
1	HHH	212	GLU
1	HHH	214	LYS

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Mol	Chain	Res	Type
2	LLL	18	LYS
2	LLL	115	SER
2	LLL	176	SER
2	LLL	205	LYS
1	III	64	LYS
1	III	85	GLU
1	III	129	LYS
1	III	150	VAL
1	III	206	LYS
1	III	212	GLU
1	III	214	LYS
2	MMM	17	GLN
2	MMM	18	LYS
2	MMM	78	LEU
2	MMM	107	LEU
2	MMM	111	LYS
2	MMM	115	SER
2	MMM	153	SER
2	MMM	167	LYS
2	MMM	176	SER
2	MMM	187	LYS
2	MMM	205	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

Of 6 ligands modelled in this entry, 2 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	ACT	III	302	-	1,3,3	3.45	1 (100%)	0,3,3	0.00	-
3	ACT	HHH	302	-	1,3,3	3.78	1 (100%)	0,3,3	0.00	-
3	ACT	HHH	301	-	1,3,3	3.23	1 (100%)	0,3,3	0.00	-
3	ACT	III	301	-	1,3,3	3.51	1 (100%)	0,3,3	0.00	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	HHH	302	ACT	CH3-C	3.78	1.53	1.48
3	III	301	ACT	CH3-C	3.51	1.53	1.48
3	III	302	ACT	CH3-C	3.45	1.53	1.48
3	HHH	301	ACT	CH3-C	3.23	1.52	1.48

There are no bond angle outliers.

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	HHH	221/233 (94%)	0.37	8 (3%) 42 45	27, 37, 61, 98	0
1	III	221/233 (94%)	0.39	8 (3%) 42 45	28, 36, 57, 93	0
2	LLL	213/220 (96%)	0.45	10 (4%) 31 34	32, 46, 71, 83	0
2	MMM	212/220 (96%)	0.72	20 (9%) 8 9	31, 52, 78, 87	0
All	All	867/906 (95%)	0.48	46 (5%) 26 29	27, 41, 70, 98	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	III	131	THR	8.0
1	HHH	130	SER	7.8
1	III	132	SER	7.6
2	LLL	107	LEU	6.0
2	MMM	107	LEU	5.5
1	HHH	131	THR	5.4
2	MMM	104	LEU	5.2
2	MMM	13	ALA	5.1
1	HHH	129	LYS	5.1
1	III	130	SER	4.8
2	MMM	210	THR	4.7
2	MMM	18	LYS	4.7
2	MMM	77	GLY	4.2
2	MMM	106	VAL	4.0
2	LLL	210	THR	3.8
2	MMM	62	PHE	3.8
1	III	133	GLY	3.5
2	MMM	156	VAL	3.5
1	HHH	128	SER	3.4
2	MMM	59	PRO	3.3
2	LLL	56	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
2	LLL	211	GLU	3.3
2	MMM	75	ILE	3.3
2	MMM	19	VAL	3.2
1	HHH	132	SER	3.1
2	LLL	155	PRO	3.1
2	MMM	105	THR	2.9
2	MMM	141	TYR	2.8
2	MMM	71	ALA	2.7
1	III	129	LYS	2.7
2	MMM	15	PRO	2.6
2	MMM	17	GLN	2.5
1	HHH	193	THR	2.5
2	LLL	57	GLY	2.5
2	MMM	76	THR	2.5
1	III	128	SER	2.4
1	HHH	127	SER	2.4
1	III	190	GLY	2.4
2	MMM	56	ALA	2.3
2	MMM	11	VAL	2.2
1	HHH	164[A]	HIS	2.2
2	LLL	111	LYS	2.2
2	LLL	173	TYR	2.1
2	LLL	15	PRO	2.1
1	III	164[A]	HIS	2.0
2	LLL	110	PRO	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, 95^{th} 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
3	ACT	HHH	301	4/4	0.87	0.12	50,52,52,53	0
3	ACT	HHH	302	4/4	0.88	0.20	63,63,65,66	0
3	ACT	III	302	4/4	0.93	0.18	52,53,53,57	0
3	ACT	III	301	4/4	0.96	0.14	56,58,59,59	0
4	CL	HHH	303	1/1	0.98	0.20	34,34,34,34	0
4	CL	III	303	1/1	0.98	0.18	36,36,36,36	0

6.5 Other polymers (i)

There are no such residues in this entry.