



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:50 PM GMT

PDB ID : 3V5L
Title : Crystal Structure of Interleukin-2 Inducible T-cell Kinase Itk Catalytic Domain with Thienopyrazolylindole Inhibitor 542
Authors : McLean, L.R.; Zhang, Y.
Deposited on : 2011-12-16
Resolution : 1.86 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

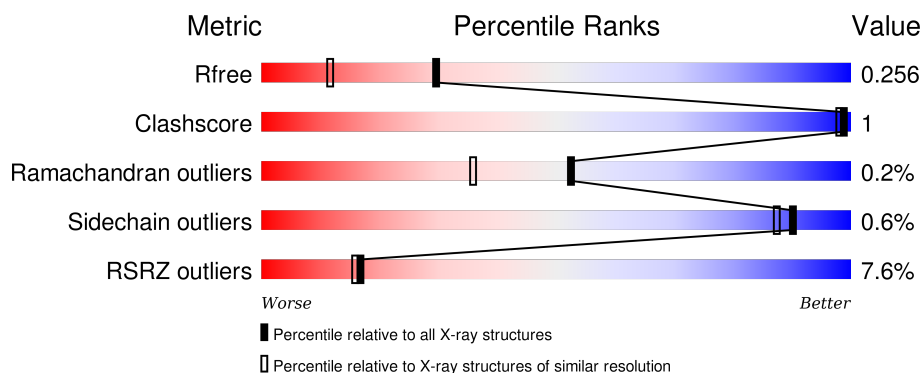
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	266	<div> <div>9%</div> <div>89%</div> <div>10%</div> </div>
1	B	266	<div> <div>8%</div> <div>90%</div> <div>9%</div> </div>
1	C	266	<div> <div>3%</div> <div>88%</div> <div>8%</div> </div>
1	D	266	<div> <div>8%</div> <div>88%</div> <div>8%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8085 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.

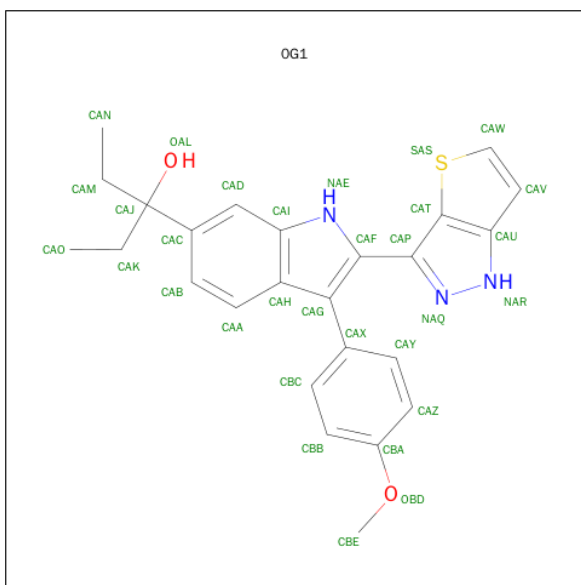
- Molecule 1 is a protein called Tyrosine-protein kinase ITK/TSK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	0	0	0
			1853	1193	306	338	16			
1	B	241	Total	C	N	O	S	0	0	0
			1860	1200	304	340	16			
1	C	244	Total	C	N	O	S	0	0	0
			1904	1223	316	348	17			
1	D	246	Total	C	N	O	S	0	0	0
			1915	1228	317	354	16			

There are 8 discrepancies between the modelled and reference sequences:

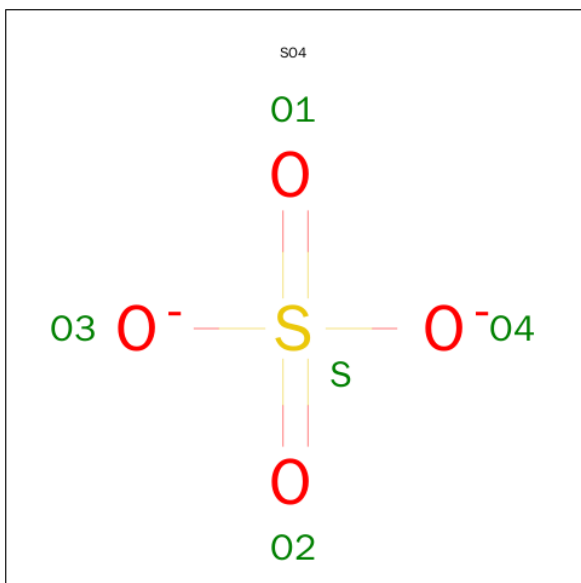
Chain	Residue	Modelled	Actual	Comment	Reference
A	355	GLY	-	EXPRESSION TAG	UNP Q08881
A	356	SER	-	EXPRESSION TAG	UNP Q08881
B	355	GLY	-	EXPRESSION TAG	UNP Q08881
B	356	SER	-	EXPRESSION TAG	UNP Q08881
C	355	GLY	-	EXPRESSION TAG	UNP Q08881
C	356	SER	-	EXPRESSION TAG	UNP Q08881
D	355	GLY	-	EXPRESSION TAG	UNP Q08881
D	356	SER	-	EXPRESSION TAG	UNP Q08881

- Molecule 2 is 3-[3-(4-METHOXYPHENYL)-2-(1H-THIENO[3,2-C]PYRAZOL-3-YL)-1H-INDOL-6-YL]PENTAN-3-OL (three-letter code: 0G1) (formula: C₂₅H₂₅N₃O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 31	C 25	N 3	O 2	S 1	0	0
2	B	1	Total 31	C 25	N 3	O 2	S 1	0	0
2	C	1	Total 31	C 25	N 3	O 2	S 1	0	0
2	D	1	Total 31	C 25	N 3	O 2	S 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		

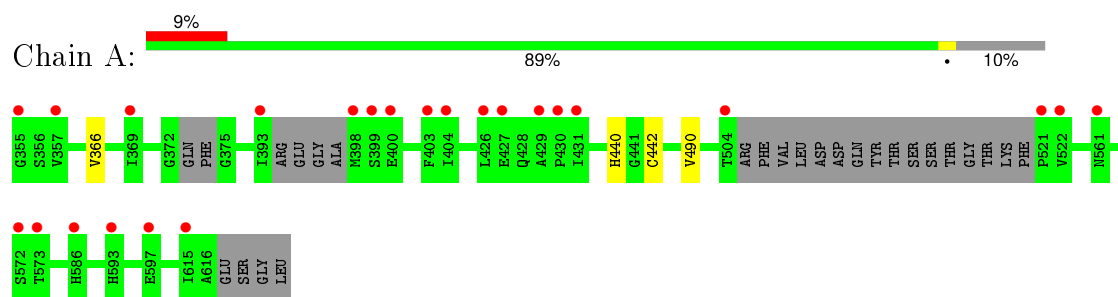
- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	86	Total	O		0	0
			86	86			
4	B	119	Total	O		0	0
			119	119			
4	C	122	Total	O		0	0
			122	122			
4	D	97	Total	O		0	0
			97	97			

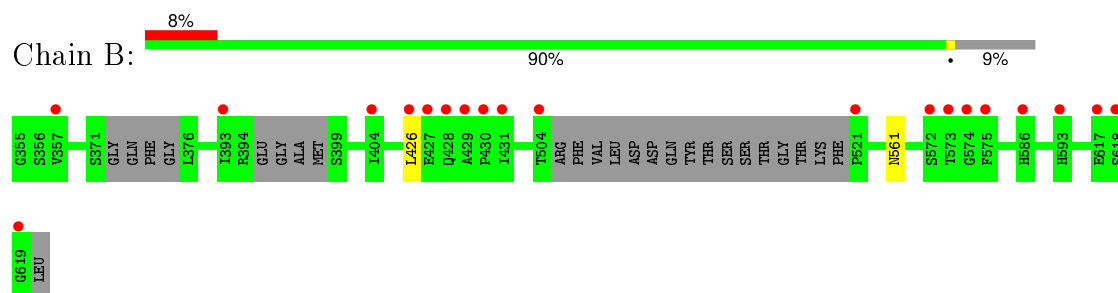
3 Residue-property plots [i](#)

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

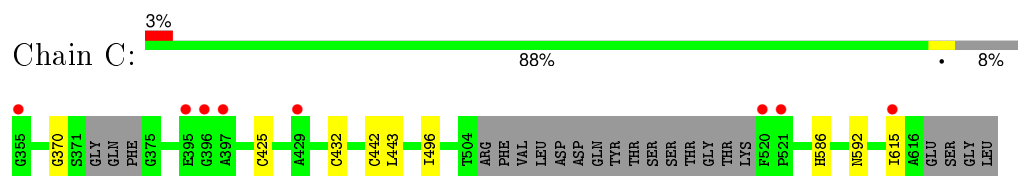
- Molecule 1: Tyrosine-protein kinase ITK/TSK



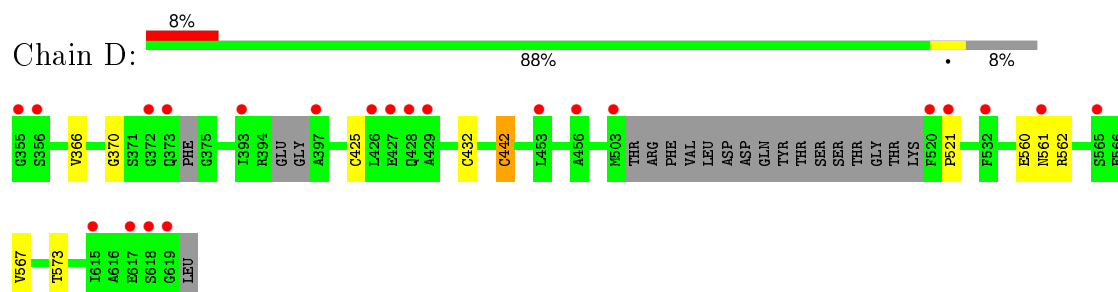
- Molecule 1: Tyrosine-protein kinase ITK/TSK



- Molecule 1: Tyrosine-protein kinase ITK/TSK



- Molecule 1: Tyrosine-protein kinase ITK/TSK



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.97Å 68.91Å 140.03Å 90.00° 100.52° 90.00°	Depositor
Resolution (Å)	47.58 – 1.86 44.42 – 1.86	Depositor EDS
% Data completeness (in resolution range)	98.1 (47.58-1.86) 98.7 (44.42-1.86)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 1.87Å)	Xtriage
Refinement program	BUSTER 2.9.1	Depositor
R, R_{free}	0.232 , 0.252 0.235 , 0.256	Depositor DCC
R_{free} test set	5316 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 106570 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8085	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.98 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.3986e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, OG1

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	0.38	0/1894	0.56	0/2561
1	B	0.38	0/1901	0.56	0/2572
1	C	0.37	0/1946	0.56	0/2631
1	D	0.38	0/1956	0.58	0/2643
All	All	0.38	0/7697	0.56	0/10407

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	1853	0	1776	3	0
1	B	1860	0	1794	1	0
1	C	1904	0	1849	4	0
1	D	1915	0	1842	6	0
2	A	31	0	25	1	0
2	B	31	0	25	0	0
2	C	31	0	25	1	0
2	D	31	0	25	2	0
3	B	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	86	0	0	0	0
4	B	119	0	0	0	0
4	C	122	0	0	0	0
4	D	97	0	0	0	0
All	All	8085	0	7361	12	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 1.

All (12) 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:C:370:GLY:HA3	2:C:701:0G1:H6	1.93	0.50
1:C:425:CYS:HB3	1:C:432:CYS:SG	2.57	0.45
1:D:442:CYS:HB3	2:D:701:0G1:H4	1.99	0.44
1:D:370:GLY:HA3	2:D:701:0G1:H6	1.99	0.43
1:A:442:CYS:HB3	2:A:701:0G1:H4	2.01	0.43
1:D:560:GLU:HA	1:D:561:ASN:HA	1.75	0.42
1:B:561:ASN:HD22	1:D:573:THR:HG22	1.84	0.42
1:D:425:CYS:HB3	1:D:432:CYS:SG	2.60	0.41
1:A:440:HIS:HB2	1:A:490:VAL:HB	2.02	0.41
1:C:586:HIS:HB3	1:C:615:ILE:HD12	2.02	0.41
1:A:366:VAL:HG11	1:D:366:VAL:HG11	2.03	0.40
1:C:443:LEU:HD13	1:C:496:ILE:HD12	2.03	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	232/266 (87%)	227 (98%)	5 (2%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	233/266 (88%)	229 (98%)	4 (2%)	0	100	100
1	C	238/266 (90%)	235 (99%)	3 (1%)	0	100	100
1	D	238/266 (90%)	230 (97%)	6 (2%)	2 (1%)	24	9
All	All	941/1064 (88%)	921 (98%)	18 (2%)	2 (0%)	52	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	521	PRO
1	D	562	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	192/233 (82%)	192 (100%)	0	100	100
1	B	196/233 (84%)	195 (100%)	1 (0%)	92	90
1	C	202/233 (87%)	200 (99%)	2 (1%)	82	76
1	D	201/233 (86%)	199 (99%)	2 (1%)	82	76
All	All	791/932 (85%)	786 (99%)	5 (1%)	90	87

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	426	LEU
1	C	442	CYS
1	C	592	ASN
1	D	442	CYS
1	D	567	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	611	GLN
1	B	378	HIS
1	B	561	ASN
1	B	589	GLN
1	B	592	ASN
1	C	378	HIS
1	C	494	GLN
1	C	564	ASN
1	C	592	ASN
1	C	611	GLN
1	D	378	HIS
1	D	494	GLN
1	D	592	ASN
1	D	611	GLN

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](#)

5 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	0G1	A	701	-	29,35,35	2.49	4 (13%)	23,52,52	1.26	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	0G1	B	701	-	29,35,35	2.47	3 (10%)	23,52,52	1.26	2 (8%)
3	SO4	B	702	-	4,4,4	0.17	0	6,6,6	0.10	0
2	0G1	C	701	-	29,35,35	2.45	4 (13%)	23,52,52	1.26	2 (8%)
2	0G1	D	701	-	29,35,35	2.48	3 (10%)	23,52,52	1.23	2 (8%)

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	0G1	A	701	-	-	0/18/22/22	0/5/5/5
2	0G1	B	701	-	-	0/18/22/22	0/5/5/5
3	SO4	B	702	-	-	0/0/0/0	0/0/0/0
2	0G1	C	701	-	-	0/18/22/22	0/5/5/5
2	0G1	D	701	-	-	0/18/22/22	0/5/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	0G1	CAG-CAX	-8.75	1.39	1.49
2	D	701	0G1	CAG-CAX	-8.71	1.39	1.49
2	C	701	0G1	CAG-CAX	-8.67	1.39	1.49
2	B	701	0G1	CAG-CAX	-8.65	1.39	1.49
2	B	701	0G1	NAR-NAQ	-7.02	1.23	1.37
2	D	701	0G1	NAR-NAQ	-6.97	1.24	1.37
2	A	701	0G1	NAR-NAQ	-6.97	1.24	1.37
2	C	701	0G1	NAR-NAQ	-6.97	1.24	1.37
2	B	701	0G1	CAP-CAF	-5.34	1.41	1.49
2	D	701	0G1	CAP-CAF	-5.29	1.41	1.49
2	A	701	0G1	CAP-CAF	-5.27	1.41	1.49
2	C	701	0G1	CAP-CAF	-5.05	1.41	1.49
2	C	701	0G1	CAJ-CAC	2.10	1.55	1.53
2	A	701	0G1	CAJ-CAC	2.20	1.55	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	0G1	CBE-OBD-CBA	-3.45	109.44	117.51
2	C	701	0G1	CBE-OBD-CBA	-3.22	109.98	117.51
2	A	701	0G1	CBE-OBD-CBA	-3.15	110.13	117.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	701	0G1	CBE-OBD-CBA	-2.84	110.86	117.51
2	B	701	0G1	CAF-NAE-CAI	3.48	111.00	103.94
2	D	701	0G1	CAF-NAE-CAI	3.52	111.09	103.94
2	A	701	0G1	CAF-NAE-CAI	3.61	111.27	103.94
2	C	701	0G1	CAF-NAE-CAI	3.71	111.47	103.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	0G1	1	0
2	C	701	0G1	1	0
2	D	701	0G1	2	0

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, 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	240/266 (90%)	0.51	24 (10%) 9 9	16, 30, 50, 69	0
1	B	241/266 (90%)	0.38	20 (8%) 14 14	13, 25, 46, 65	0
1	C	244/266 (91%)	0.22	8 (3%) 50 47	12, 23, 41, 64	0
1	D	246/266 (92%)	0.45	22 (8%) 12 11	14, 28, 47, 71	0
All	All	971/1064 (91%)	0.39	74 (7%) 17 16	12, 27, 47, 71	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	520	PHE	8.5
1	B	429	ALA	7.9
1	D	397	ALA	6.5
1	C	396	GLY	6.4
1	A	429	ALA	6.4
1	C	397	ALA	6.1
1	A	521	PRO	5.6
1	B	573	THR	5.4
1	D	561	ASN	5.3
1	D	618	SER	4.7
1	B	426	LEU	4.7
1	D	372	GLY	4.6
1	A	427	GLU	4.5
1	C	520	PHE	4.4
1	D	521	PRO	4.4
1	B	618	SER	4.3
1	D	429	ALA	4.3
1	B	427	GLU	4.2
1	B	575	PHE	4.1
1	A	430	PRO	3.5
1	C	355	GLY	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	355	GLY	3.3
1	B	428	GLN	3.2
1	C	521	PRO	3.2
1	A	399	SER	3.2
1	A	573	THR	3.2
1	D	373	GLN	3.1
1	A	572	SER	3.0
1	A	355	GLY	3.0
1	B	521	PRO	2.9
1	D	619	GLY	2.8
1	B	572	SER	2.8
1	A	398	MET	2.7
1	A	393	ILE	2.7
1	C	395	GLU	2.7
1	B	617	GLU	2.7
1	D	426	LEU	2.6
1	A	404	ILE	2.6
1	A	615	ILE	2.6
1	D	532	PHE	2.6
1	A	426	LEU	2.6
1	B	393	ILE	2.6
1	D	503	MET	2.5
1	A	431	ILE	2.5
1	B	619	GLY	2.5
1	C	429	ALA	2.5
1	D	428	GLN	2.4
1	B	404	ILE	2.4
1	B	431	ILE	2.4
1	D	617	GLU	2.4
1	A	400	GLU	2.4
1	A	522	VAL	2.4
1	A	586	HIS	2.4
1	A	593	HIS	2.3
1	A	357	VAL	2.3
1	C	615	ILE	2.3
1	A	561	ASN	2.2
1	B	574	GLY	2.2
1	A	403	PHE	2.2
1	D	393	ILE	2.2
1	D	453	LEU	2.2
1	B	430	PRO	2.1
1	D	356	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	615	ILE	2.1
1	D	565	SER	2.1
1	B	504	THR	2.1
1	D	456	ALA	2.1
1	B	593	HIS	2.0
1	D	427	GLU	2.0
1	A	369	ILE	2.0
1	B	586	HIS	2.0
1	A	504	THR	2.0
1	B	357	VAL	2.0
1	A	597	GLU	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 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
2	0G1	B	701	31/31	0.95	0.12	0.25	13,18,40,58	0
2	0G1	C	701	31/31	0.97	0.11	-0.03	11,17,36,99	0
2	0G1	A	701	31/31	0.95	0.12	-0.06	16,24,37,43	0
3	SO4	B	702	5/5	0.99	0.10	-0.89	24,29,29,30	0
2	0G1	D	701	31/31	0.96	0.09	-1.12	14,21,35,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.