



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 04:31 AM EDT

PDB ID : 3IV1
Title : Coiled-coil domain of tumor susceptibility gene 101
Authors : Neculai, D.; Avvakumov, G.V.; Wernimont, A.K.; Xue, S.; Walker, J.R.; Li, Y.; Weigelt, J.; Bountra, C.; Arrowsmith, C.H.; Edwards, A.M.; Bochkarev, A.; Dhe-Paganon, S.; Structural Genomics Consortium (SGC)
Deposited on : 2009-08-31
Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 1.20.1
EDS : 2.37.1
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

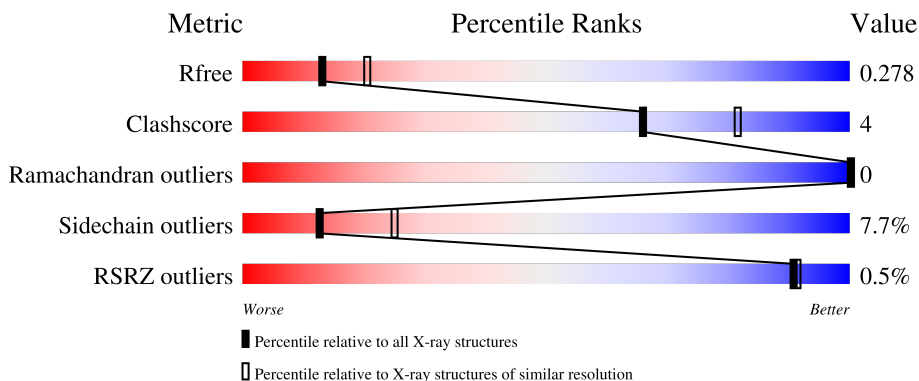
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	78	
1	B	78	
1	C	78	
1	D	78	
1	E	78	

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Mol	Chain	Length	Quality of chain
1	F	78	 85% 15%
1	G	78	 92% 8%
1	H	78	 % 86% 13% •

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5199 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 Tumor susceptibility gene 101 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	78	638	391	113	130	4	0	1	0
1	B	78	638	391	113	130	4	0	1	0
1	C	78	638	391	113	130	4	0	1	0
1	D	78	638	391	113	130	4	0	1	0
1	E	78	638	391	113	130	4	0	1	0
1	F	78	638	391	113	130	4	0	1	0
1	G	78	630	386	112	129	3	0	0	0
1	H	78	638	391	113	130	4	0	1	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	227	GLY	-	EXPRESSION TAG	UNP Q99816
A	228	SER	-	EXPRESSION TAG	UNP Q99816
B	227	GLY	-	EXPRESSION TAG	UNP Q99816
B	228	SER	-	EXPRESSION TAG	UNP Q99816
C	227	GLY	-	EXPRESSION TAG	UNP Q99816
C	228	SER	-	EXPRESSION TAG	UNP Q99816
D	227	GLY	-	EXPRESSION TAG	UNP Q99816
D	228	SER	-	EXPRESSION TAG	UNP Q99816
E	227	GLY	-	EXPRESSION TAG	UNP Q99816
E	228	SER	-	EXPRESSION TAG	UNP Q99816
F	227	GLY	-	EXPRESSION TAG	UNP Q99816
F	228	SER	-	EXPRESSION TAG	UNP Q99816
G	227	GLY	-	EXPRESSION TAG	UNP Q99816

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Chain	Residue	Modelled	Actual	Comment	Reference
G	228	SER	-	EXPRESSION TAG	UNP Q99816
H	227	GLY	-	EXPRESSION TAG	UNP Q99816
H	228	SER	-	EXPRESSION TAG	UNP Q99816

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	O S	0	0
			5	4 1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		
3	C	2	Total	Cl	0	0
			2	2		
3	D	2	Total	Cl	0	0
			2	2		
3	E	2	Total	Cl	0	0
			2	2		
3	F	1	Total	Cl	0	0
			1	1		
3	G	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	1	Total	Cl	0	0
			1	1		

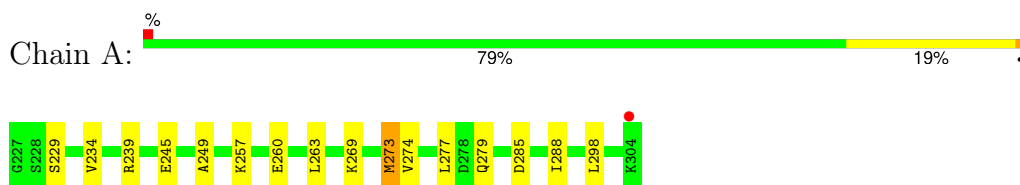
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	11	Total	O	0	0
			11	11		
4	B	13	Total	O	0	0
			13	13		
4	C	12	Total	O	0	0
			12	12		
4	D	9	Total	O	0	0
			9	9		
4	E	13	Total	O	0	0
			13	13		
4	F	10	Total	O	0	0
			10	10		
4	G	7	Total	O	0	0
			7	7		
4	H	12	Total	O	0	0
			12	12		

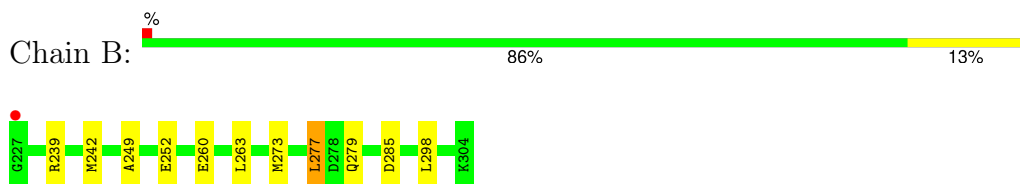
3 Residue-property plots [i](#)

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.

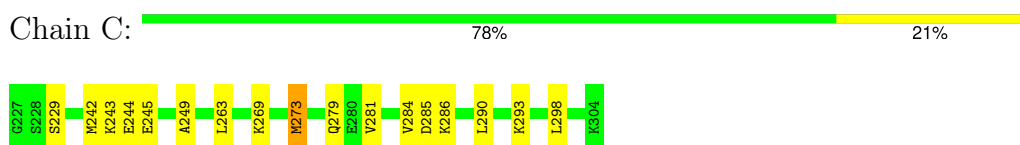
- Molecule 1: Tumor susceptibility gene 101 protein



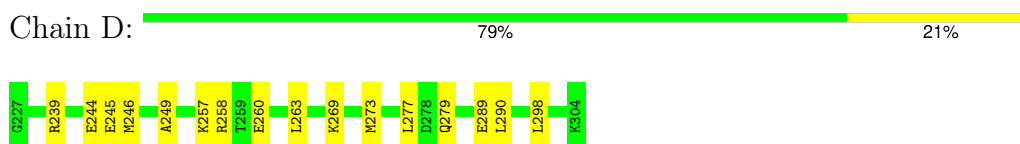
- Molecule 1: Tumor susceptibility gene 101 protein



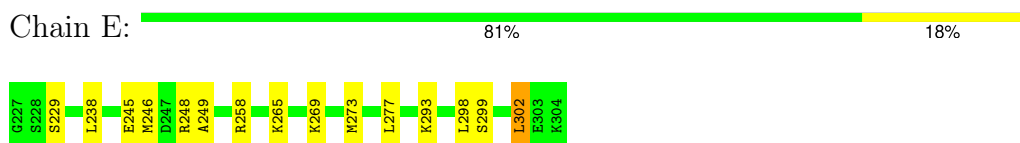
- Molecule 1: Tumor susceptibility gene 101 protein




- Molecule 1: Tumor susceptibility gene 101 protein



- Molecule 1: Tumor susceptibility gene 101 protein



- Molecule 1: Tumor susceptibility gene 101 protein

Chain F:  85% 15%




- Molecule 1: Tumor susceptibility gene 101 protein

Chain G:  92% 8%



- Molecule 1: Tumor susceptibility gene 101 protein

Chain H:  % 86% 13%



4 Data and refinement statistics i

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	56.29Å 56.29Å 341.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.75 – 2.50 48.75 – 2.42	Depositor EDS
% Data completeness (in resolution range)	(Not available) (48.75-2.50) 99.8 (48.75-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.05 (at 2.42Å)	Xtrriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.228 , 0.277 0.226 , 0.278	Depositor DCC
R_{free} test set	1286 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtrriage
Anisotropy	0.488	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 28.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.487 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5199	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.17 % 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 1.1573e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: CL, SO4

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	0.49	0/637	0.64	0/840
1	B	0.51	0/637	0.62	0/840
1	C	0.49	0/637	0.64	0/840
1	D	0.50	0/637	0.67	0/840
1	E	0.53	1/637 (0.2%)	0.65	0/840
1	F	0.48	0/637	0.62	0/840
1	G	0.47	0/629	0.63	0/830
1	H	0.50	0/637	0.66	0/840
All	All	0.50	1/5088 (0.0%)	0.64	0/6710

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	246	MSE	SE-CE	-5.03	1.65	1.95

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	638	0	656	12	0
1	B	638	0	656	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	638	0	656	14	0
1	D	638	0	656	12	0
1	E	638	0	656	7	0
1	F	638	0	656	7	0
1	G	630	0	648	2	0
1	H	638	0	656	5	0
2	A	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	11	0	0	0	0
4	B	13	0	0	0	0
4	C	12	0	0	1	0
4	D	9	0	0	0	0
4	E	13	0	0	0	0
4	F	10	0	0	0	0
4	G	7	0	0	0	0
4	H	12	0	0	0	0
All	All	5199	0	5240	41	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 4.

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:B:277:LEU:HD11	1:D:245:GLU:HG3	1.36	1.06
1:C:281:VAL:HG13	1:D:239:ARG:HG2	1.53	0.88
1:C:273[A]:MSE:HE1	1:D:246:MSE:SE	2.28	0.84
1:B:273[B]:MSE:SE	1:D:249:ALA:HB2	2.38	0.73
1:G:249:ALA:HB2	1:H:273[A]:MSE:SE	2.44	0.68
1:E:273[A]:MSE:SE	1:F:249:ALA:HB2	2.47	0.63
1:C:285:ASP:OD2	1:D:239:ARG:HD2	2.01	0.61
1:H:288:ILE:HD12	1:H:292:LYS:HD2	1.89	0.55
1:B:263:LEU:HD21	1:C:263:LEU:HD11	1.88	0.55
1:A:273[A]:MSE:HG3	1:A:274:VAL:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ASP:OD1	1:B:239:ARG:HD2	2.09	0.53
1:A:239:ARG:HD2	1:B:285:ASP:OD1	2.12	0.49
1:E:249:ALA:N	1:F:273[B]:MSE:HE1	2.27	0.49
1:D:269:LYS:O	1:D:273[B]:MSE:HG3	2.13	0.48
1:C:269:LYS:O	1:C:273[B]:MSE:HG3	2.13	0.47
1:C:273[A]:MSE:CE	1:D:246:MSE:SE	3.06	0.47
1:F:269:LYS:O	1:F:273[B]:MSE:HG3	2.14	0.47
1:A:249:ALA:N	1:C:273[B]:MSE:HE1	2.31	0.46
1:A:273[A]:MSE:SE	1:C:249:ALA:HB2	2.66	0.46
1:C:242:MSE:HE1	1:D:277:LEU:HD23	1.99	0.45
1:A:263:LEU:HD11	1:D:263:LEU:HD21	1.97	0.45
1:C:243:LYS:HG3	4:C:100:HOH:O	2.16	0.45
1:B:242:MSE:SE	1:C:242:MSE:HG3	2.67	0.45
1:E:299:SER:O	1:E:302:LEU:HB2	2.17	0.44
1:D:257:LYS:HA	1:D:260:GLU:HG2	2.00	0.43
1:A:269:LYS:O	1:A:273[B]:MSE:HG3	2.19	0.43
1:B:249:ALA:N	1:D:273[B]:MSE:HE1	2.34	0.43
1:E:277:LEU:HD11	1:F:245:GLU:CB	2.49	0.42
1:B:252:GLU:OE1	1:D:269:LYS:HD2	2.20	0.42
1:E:269:LYS:O	1:E:273[B]:MSE:HG3	2.19	0.42
1:H:269:LYS:O	1:H:273[B]:MSE:HG3	2.19	0.42
1:A:273[A]:MSE:HE2	1:A:273[A]:MSE:HB2	1.80	0.42
1:A:234:VAL:HG13	1:C:284:VAL:HG22	2.00	0.42
1:A:277:LEU:HD11	1:C:245:GLU:CB	2.50	0.41
1:E:245:GLU:OE2	1:F:276:ARG:HD2	2.21	0.41
1:F:264:LYS:HD2	1:F:268:GLN:NE2	2.35	0.41
1:E:238:LEU:HB2	1:F:284:VAL:HG21	2.02	0.41
1:H:231:ILE:HG13	1:H:232:SER:N	2.34	0.41
1:G:238:LEU:HB2	1:H:284:VAL:HG21	2.03	0.40
1:A:245:GLU:O	1:C:273[B]:MSE:HE1	2.22	0.40
1:A:257:LYS:O	1:A:260:GLU:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	77/78 (99%)	77 (100%)	0	0	100	100
1	B	77/78 (99%)	77 (100%)	0	0	100	100
1	C	77/78 (99%)	77 (100%)	0	0	100	100
1	D	77/78 (99%)	77 (100%)	0	0	100	100
1	E	77/78 (99%)	77 (100%)	0	0	100	100
1	F	77/78 (99%)	76 (99%)	1 (1%)	0	100	100
1	G	76/78 (97%)	76 (100%)	0	0	100	100
1	H	77/78 (99%)	77 (100%)	0	0	100	100
All	All	615/624 (99%)	614 (100%)	1 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	71/67 (106%)	65 (92%)	6 (8%)	10	21
1	B	71/67 (106%)	67 (94%)	4 (6%)	21	40
1	C	71/67 (106%)	62 (87%)	9 (13%)	4	8
1	D	71/67 (106%)	65 (92%)	6 (8%)	10	21
1	E	71/67 (106%)	64 (90%)	7 (10%)	8	15
1	F	71/67 (106%)	67 (94%)	4 (6%)	21	40
1	G	70/67 (104%)	66 (94%)	4 (6%)	20	39
1	H	71/67 (106%)	66 (93%)	5 (7%)	15	29
All	All	567/536 (106%)	522 (92%)	45 (8%)	13	24

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	229	SER
1	A	273[A]	MSE
1	A	273[B]	MSE
1	A	279	GLN
1	A	288	ILE
1	A	298	LEU
1	B	260	GLU
1	B	277	LEU
1	B	279	GLN
1	B	298	LEU
1	C	229	SER
1	C	244	GLU
1	C	273[A]	MSE
1	C	273[B]	MSE
1	C	279	GLN
1	C	286	LYS
1	C	290	LEU
1	C	293	LYS
1	C	298	LEU
1	D	244	GLU
1	D	258	ARG
1	D	279	GLN
1	D	289	GLU
1	D	290	LEU
1	D	298	LEU
1	E	229	SER
1	E	248	ARG
1	E	258	ARG
1	E	265	LYS
1	E	293	LYS
1	E	298	LEU
1	E	302	LEU
1	F	229	SER
1	F	241	ARG
1	F	279	GLN
1	F	298	LEU
1	G	241	ARG
1	G	257	LYS
1	G	279	GLN
1	G	298	LEU
1	H	244	GLU
1	H	265	LYS
1	H	288	ILE

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Mol	Chain	Res	Type
1	H	289	GLU
1	H	298	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	254	ASN
1	B	254	ASN
1	C	268	GLN
1	F	268	GLN
1	G	268	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 11 are monoatomic - leaving 1 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	$\# Z > 2$
2	SO4	A	601	-	4,4,4	0.28	0	6,6,6	0.10	0

There are no bond length outliers.

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 [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	75/78 (96%)	-0.42	1 (1%) 77 79	18, 37, 52, 82	0
1	B	75/78 (96%)	-0.43	1 (1%) 77 79	19, 33, 57, 66	0
1	C	75/78 (96%)	-0.37	0 100 100	17, 34, 55, 76	0
1	D	75/78 (96%)	-0.39	0 100 100	20, 35, 56, 66	0
1	E	75/78 (96%)	-0.45	0 100 100	19, 35, 53, 68	0
1	F	75/78 (96%)	-0.48	0 100 100	20, 35, 56, 65	0
1	G	75/78 (96%)	-0.43	0 100 100	20, 35, 55, 70	0
1	H	75/78 (96%)	-0.42	1 (1%) 77 79	18, 35, 56, 93	0
All	All	600/624 (96%)	-0.42	3 (0%) 91 91	17, 35, 56, 93	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	227	GLY	2.3
1	B	227	GLY	2.2
1	A	304	LYS	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
3	CL	D	601	1/1	0.82	0.23	57,57,57,57	0
3	CL	A	602	1/1	0.94	0.10	61,61,61,61	0
3	CL	C	601	1/1	0.96	0.29	57,57,57,57	0
3	CL	C	305	1/1	0.96	0.22	58,58,58,58	0
2	SO4	A	601	5/5	0.96	0.10	85,90,90,91	0
3	CL	D	602	1/1	0.96	0.17	55,55,55,55	0
3	CL	H	601	1/1	0.96	0.10	64,64,64,64	0
3	CL	E	601	1/1	0.97	0.14	44,44,44,44	0
3	CL	F	601	1/1	0.97	0.22	60,60,60,60	0
3	CL	B	602	1/1	0.97	0.12	53,53,53,53	0
3	CL	G	601	1/1	0.99	0.17	51,51,51,51	0
3	CL	E	602	1/1	0.99	0.15	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.