



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 08:08 am BST

PDB ID : 5T4Y
Title : Crystal structure of BT1762-1763
Authors : van den Berg, B.
Deposited on : 2016-08-30
Resolution : 3.10 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

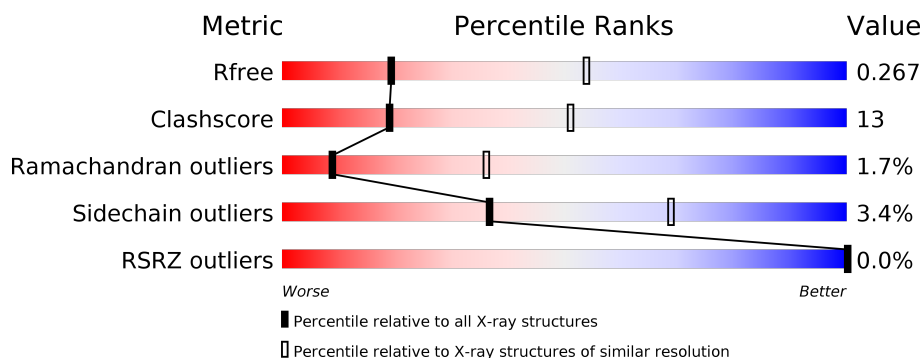
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 $\leq 5\%$. 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	576	
1	B	576	
2	C	1041	
2	D	1041	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21727 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 SusD homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	2	0
			4450	2818	737	874	21			
1	B	553	Total	C	N	O	S	0	2	0
			4460	2824	740	875	21			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	553	HIS	-	expression tag	UNP Q8A6W4
A	554	HIS	-	expression tag	UNP Q8A6W4
A	555	HIS	-	expression tag	UNP Q8A6W4
A	556	HIS	-	expression tag	UNP Q8A6W4
A	557	HIS	-	expression tag	UNP Q8A6W4
A	558	HIS	-	expression tag	UNP Q8A6W4
B	553	HIS	-	expression tag	UNP Q8A6W4
B	554	HIS	-	expression tag	UNP Q8A6W4
B	555	HIS	-	expression tag	UNP Q8A6W4
B	556	HIS	-	expression tag	UNP Q8A6W4
B	557	HIS	-	expression tag	UNP Q8A6W4
B	558	HIS	-	expression tag	UNP Q8A6W4

- Molecule 2 is a protein called SusC homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	807	Total	C	N	O	S	0	0	0
			6406	4057	1089	1241	19			
2	C	807	Total	C	N	O	S	0	0	0
			6406	4057	1089	1241	19			

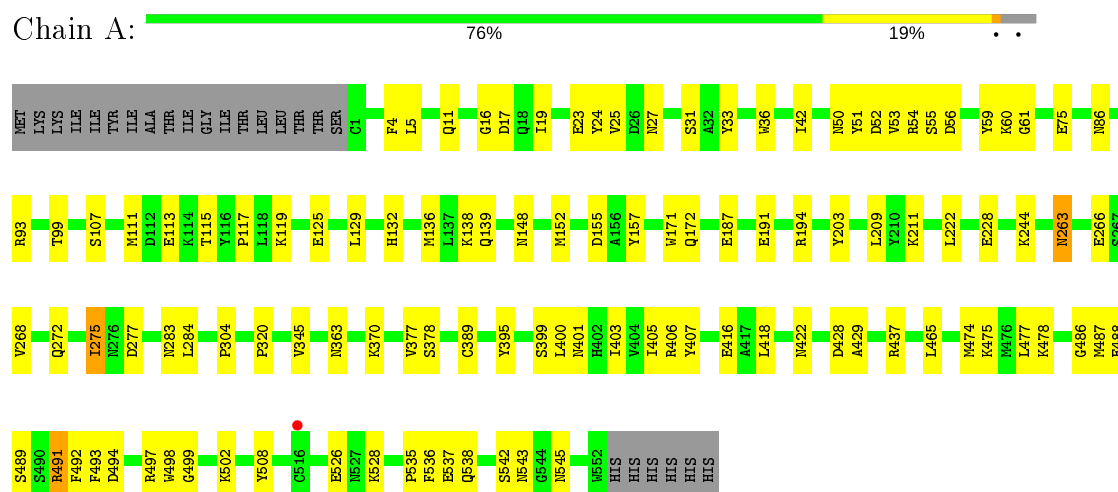
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total 2	Mg 2	0	0
3	A	2	Total 2	Mg 2	0	0
3	C	1	Total 1	Mg 1	0	0

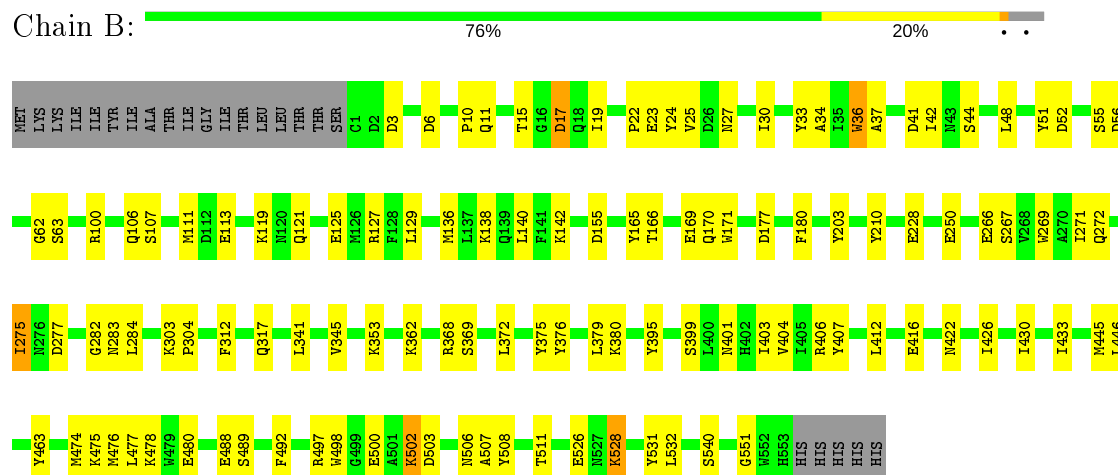
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: SusD homolog



• Molecule 1: SusD homolog



• Molecule 2: SusC homolog



LEU	TTR	ILE	ILE	ASP	LEU	THR	ASP	THR	MET
Q226	Q236	Q241	Q242	Q246	Q255	Q256	Q257	Q258	Q259
K335	D336	F339	D340	R341	R345	M346	K351	L352	L353
R421	Y422	T423	W424	W425	W426	W427	L435	T436	P437
K523	E524	E525	E526	E528	E531	E532	E533	E534	E535
Q603	E604	M605	F606	M607	K608	E609	L610	W611	W612
I695	D696	F697	S698	L699	F700	E701	S702	S703	Y704
K794	S795	Y796	Y797	G798	H799	T800	Y801	Q804	L805
D895	Y902	L905	N906	H907	R910	L911	W915	P920	P925
N933	N934	E935	Q936	R937	T940	F948	L949	X950	R953
A962	Y963	Y964	S965	K966	N970	D971	A979	T984	I985
Y986	L987	E988	Y989	K990	F990	E993	E996	N997	P998
F1016									

• Molecule 2: SusC homolog



LEU	TTR	ILE	ILE	ASP	LEU	THR	ASP	THR	MET
G210	Q211	I212	A213	S219					
GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO

V220	K318	G403	R502	E604	S703	D817	L911	T1009
S221	K319	D406	G503	M605	L704	E818	L912	
K228	S320	R407	D504	K608	Y705		N913	L1012
V231	S321	R408	V505	D614	G706	H822	A914	F1016
L232	F322	N469	M506	L708	S707	T824	P925	
N233	L325	P410	I507	D815	E709	Q825	A826	
T234	Y328	R411	D516	L616	Y712	E826	L827	
Q236	Y328	E415	S520	L618	I718	A828	A828	
Y237	L331	Y422	D525	Q624	L719	R832	N933	
G238	I334	W425	I528	Q628	T720	T833	N934	
R239	K335	R426	L529	N632	G731	R834	E935	
Q243	D336	M427	T530	L633	G732	Y835	R937	
A244	T337	F428	Y533	G547	S733	R836	V938	
Y245	D338	G429	Y534	D647	R734	D837	S939	
Y246	R345	D430	M535	S648	W735	I838	T940	
N247	M346	A431	W535	G651	I736	D845	Y943	
P252	D349	Y432	G541	T656	G739	E846	K950	
N255	Y350	N434	Y546	A640	K742	R847	L951	
G258	K351	I435	G547	N642	E747	Q849	Q955	
Y259	L352	T436	A548	D647	F748	M850	L956	
N262	I353	P437	G549	S648		M851		
D262	D355	F438	N562	G651	G751	I852	S965	
N266	I356	K439	Y563	T656	Y752	P857	K966	
	L357	N442	S564	A657	L764	I865	R969	
	G360	L449	Y665	Y688		F872	R970	
V272	D450	Y451	R568	I660	I768	D873	D971	
L273	H362		Y569			L874	R972	
Y274	F363				L776	T875	R974	
L278	T364	K454	T574	L669	E777	V884	C977	
S279	R367	Q455	L575	P670	K787	D885		
K280	E370	A456	R576	F673	F788	I886	N981	
Y281	V371	P462	D578	K674		I887	L982	
L282		Y463		R675	N791	S888		
V290	P374	G466	R582	M676	G792	D889	K986	
A291	G375	T467	K585	Q677	V797	K891	S887	
D292	I377	Q468	N586	I678		K892	K986	
T293	I376	T469	H587	G679	Y801	K893	N989	
D294	I378	N470	R588	N682		S894	F990	
W295	E379	N471	Y589	I683	Q804	D895	T991	
F296	D383	G472	A590	K684	V805		G992	
T297		W483	P593	W685	G806	N901	E993	
E298	V390	M487	S594	T691	Y807	V902	E996	
R301	V304		L597	I695	I808	G903	N997	
I305	K397	E497	G598	D696	A809	F904	P998	
	P400	V498	I601	F697	D810	N906	P1003	
S313	N314	G499	T602	K701	G811	K907	V1006	
G315	G402	K500	Q603	Q702	I812	G908	N1007	
					K814	T909	I1008	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.83Å 152.09Å 253.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	130.35 – 3.10 130.35 – 2.99	Depositor EDS
% Data completeness (in resolution range)	98.9 (130.35-3.10) 98.6 (130.35-2.99)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.198 , 0.270 0.198 , 0.267	Depositor DCC
R_{free} test set	4357 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	68.3	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 56.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21727	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

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: MG

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	0.44	0/4562	0.62	2/6190 (0.0%)
1	B	0.49	1/4573 (0.0%)	0.66	1/6205 (0.0%)
2	C	0.59	8/6571 (0.1%)	0.76	4/8909 (0.0%)
2	D	0.52	0/6571	0.76	3/8909 (0.0%)
All	All	0.52	9/22277 (0.0%)	0.71	10/30213 (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
2	D	0	4

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	709	GLU	CG-CD	-6.93	1.41	1.51
2	C	565	TYR	CE1-CZ	-6.63	1.29	1.38
2	C	565	TYR	CE2-CZ	-6.15	1.30	1.38
2	C	565	TYR	CG-CD1	-6.06	1.31	1.39
1	B	36	TRP	CB-CG	-5.99	1.39	1.50

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	911	LEU	CA-CB-CG	6.11	129.35	115.30
2	D	911	LEU	CB-CG-CD2	5.82	120.89	111.00
1	A	275	ILE	CG1-CB-CG2	-5.81	98.62	111.40
2	D	449	LEU	CA-CB-CG	5.42	127.77	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	565	TYR	CA-CB-CG	5.39	123.65	113.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	317	GLU	Peptide
2	D	353	ILE	Peptide
2	D	470	ASN	Peptide
2	D	584	GLY	Peptide

5.2 Too-close contacts

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	4450	0	4219	80	0
1	B	4460	0	4227	81	0
2	C	6406	0	6058	208	0
2	D	6406	0	6058	222	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
All	All	21727	0	20562	549	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 13.

The worst 5 of 549 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)
2:D:427:MET:CE	2:C:427:MET:SD	2.35	1.12
2:D:427:MET:HE2	2:C:427:MET:SD	1.95	1.04
2:D:427:MET:HE3	2:C:427:MET:SD	2.00	1.00
1:B:275:ILE:HG22	1:B:284:LEU:HD11	1.47	0.95
2:D:365:LEU:HD13	2:D:427:MET:SD	2.12	0.90

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	552/576 (96%)	500 (91%)	48 (9%)	4 (1%)	22	57
1	B	553/576 (96%)	514 (93%)	36 (6%)	3 (0%)	29	64
2	C	805/1041 (77%)	716 (89%)	68 (8%)	21 (3%)	5	26
2	D	805/1041 (77%)	714 (89%)	72 (9%)	19 (2%)	6	27
All	All	2715/3234 (84%)	2444 (90%)	224 (8%)	47 (2%)	9	36

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	608	LYS
2	D	826	GLU
2	D	993	GLU
2	C	732	GLY
2	C	971	ASP

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	475/495 (96%)	469 (99%)	6 (1%)	69	87
1	B	476/495 (96%)	469 (98%)	7 (2%)	65	85
2	C	673/869 (77%)	644 (96%)	29 (4%)	29	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	673/869 (77%)	637 (95%)	36 (5%)	22	54
All	All	2297/2728 (84%)	2219 (97%)	78 (3%)	37	69

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	801	TYR
1	B	17	ASP
2	C	969	ARG
2	D	834	ARG
2	D	911	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	110	GLN
2	C	913	ASN
2	C	791	ASN
2	D	849	GLN
2	C	442	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

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	552/576 (95%)	-0.38	1 (0%) 95 90	47, 83, 111, 146	0
1	B	553/576 (96%)	-0.33	0 100 100	37, 65, 95, 124	0
2	C	807/1041 (77%)	-0.44	0 100 100	37, 64, 104, 150	0
2	D	807/1041 (77%)	-0.39	0 100 100	35, 71, 111, 146	0
All	All	2719/3234 (84%)	-0.39	1 (0%) 100 100	35, 70, 108, 150	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	516	CYS	2.1

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. 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	MG	A	602	1/1	0.84	0.09	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	B	602	1/1	0.94	0.17	113,113,113,113	0
3	MG	C	1101	1/1	0.96	0.22	47,47,47,47	0
3	MG	B	601	1/1	0.96	0.12	4,4,4,4	0
3	MG	A	601	1/1	0.97	0.16	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.